



Challenges of and Variations on Coupled Atomistic-Continuum Simulation

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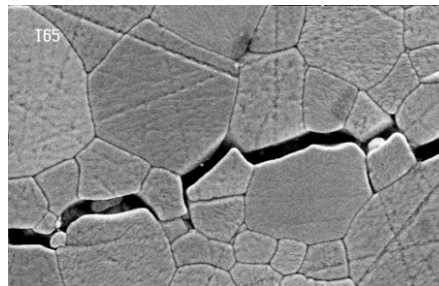
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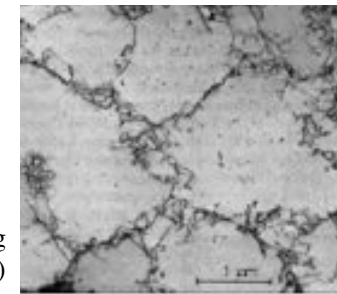
Motivation: Scale-dependent mechanical deformation

Material deformation and failure operate at various length scales:

- Brittle and ductile fracture
- Dislocation activity
- Grain boundary sliding
- Stiction, friction and wear



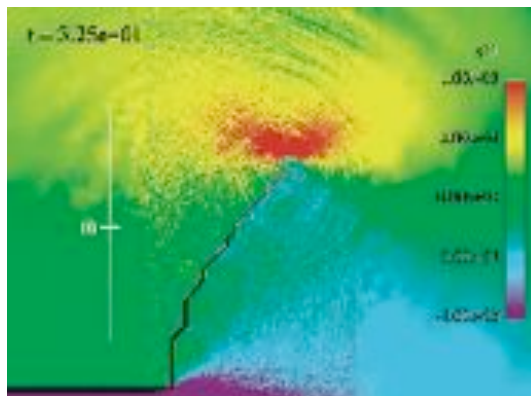
(Pferner; 1999)



(Bulatov, Tang and Zbib; 2001)

Continuum Mechanics:

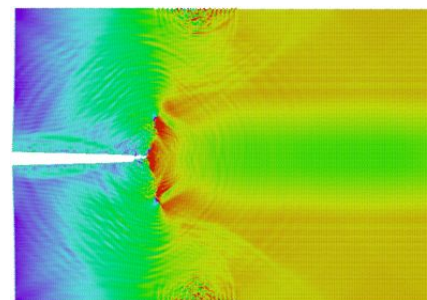
displacement, stress,
temperature, heat flux



Cohesive
surface network
simulation of
Kalthoff-
Winkler
experiment

Atomistic Simulation:

position, velocity, force



Steady-state, dynamic
crack propagation using
molecular dynamics



Motivation: Translating atomistic for engineers

The material description is very different between atomistics and continuum.

Connecting the two methods requires definitions of measures with the same physical meaning.

Such definitions are vital for

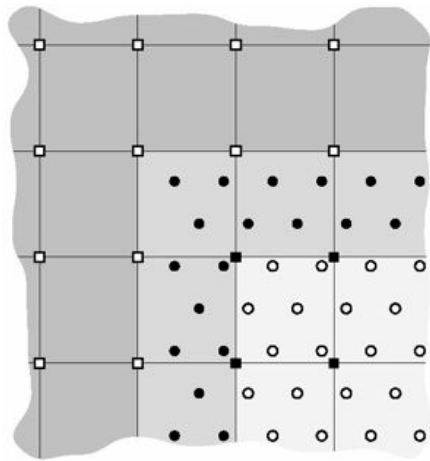
- **comparing analyses** of the same material phenomenon
- **providing interface conditions** between domains for coupled analysis

Coupling atomistic and continuum simulations requires rigorous definitions for all types of variables. For example: stress, strain, heat flux, temperature, internal state variables.

Coupling can also be accomplished through informational (hierarchical) means, *i.e.* information obtained through atomistics is used to enhance aspects of the continuum model/simulation.

One such example: using MD to construct **traction-separation relations** for cohesive surface element simulations.

Arbitrary overlapping domain formulation



Finite element mesh exists throughout the simulation region:

□ — \mathbf{U} free nodes
 ■ — $\hat{\mathbf{U}}$ nodes with displacement prescribed via **projection** from atomistics

Atoms are present in limited regions:

○ — \mathbf{Q} free atoms
 ● — $\hat{\mathbf{Q}}$ ghost atoms with displacement prescribed via **interpolation** from the continuum

System potential energy = energy in atomic regions + energy in the continuum:

$$\Pi(\mathbf{Q}, \mathbf{U}) = \Pi_{\mathbf{Q}}(\mathbf{Q}, \hat{\mathbf{Q}}(\mathbf{Q}, \mathbf{U})) + \Pi_{\mathbf{U}}(\mathbf{U}, \hat{\mathbf{U}}(\mathbf{Q}, \mathbf{U})) - \mathbf{F}_{\mathbf{Q}} \cdot \mathbf{Q} - \mathbf{F}_{\mathbf{U}} \cdot \mathbf{U}$$

Our coupling formulation is comprised of three components:

- kinematics - transfer of displacements between nodes and atoms
- coupled equilibrium equations - system energy + kinematics
- generalized Cauchy-Born rule - alter bond density to compensate for real atom-ghost atom bonds



Kinematics of quasistatic coupling

Projection

Atomistic displacements (\mathbf{Q}) are separated into the coarse scale projection and a fine scale remainder:

$$\begin{Bmatrix} \mathbf{Q} \\ \hat{\mathbf{Q}} \end{Bmatrix} = \begin{bmatrix} \mathbf{N}_{\mathbf{QU}} & \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}} \\ \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{U}} & \mathbf{N}_{\hat{\mathbf{Q}}\hat{\mathbf{U}}} \end{bmatrix} \begin{Bmatrix} \mathbf{U} \\ \hat{\mathbf{U}} \end{Bmatrix} + \begin{Bmatrix} \mathbf{Q}' \\ \mathbf{0} \end{Bmatrix}$$

For quasi-statics, \mathbf{Q}' is used as an error estimator and can be used to:

- guide mesh refinement
- track material defects
- activate adaptive lattice extension or removal

Interpolation

The continuum impacts the atomistic region(s) through the use of ghost atoms. Their displacements ($\hat{\mathbf{Q}}$), and other properties are determined through interpolation of continuum fields at ghost atom positions.

To minimize \mathbf{Q}' :

$$\hat{\mathbf{U}} = \mathbf{B}_{\hat{\mathbf{U}}\mathbf{Q}} \mathbf{Q} + \mathbf{B}_{\hat{\mathbf{U}}\mathbf{U}} \mathbf{U}$$

$$\hat{\mathbf{Q}} = \mathbf{B}_{\hat{\mathbf{Q}}\mathbf{Q}} \mathbf{Q} + \mathbf{B}_{\hat{\mathbf{Q}}\mathbf{U}} \mathbf{U}$$

$$\mathbf{M}_{\hat{\mathbf{U}}\hat{\mathbf{U}}} = \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}^T \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}$$

$$\mathbf{B}_{\hat{\mathbf{U}}\mathbf{Q}} = \mathbf{M}_{\hat{\mathbf{U}}\hat{\mathbf{U}}}^{-1} \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}^T$$

$$\mathbf{B}_{\hat{\mathbf{U}}\mathbf{U}} = -\mathbf{M}_{\hat{\mathbf{U}}\hat{\mathbf{U}}}^{-1} \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}^T \mathbf{N}_{\mathbf{Q}\mathbf{U}} = -\mathbf{B}_{\hat{\mathbf{U}}\mathbf{Q}} \mathbf{N}_{\mathbf{Q}\mathbf{U}}$$

$$\mathbf{B}_{\hat{\mathbf{Q}}\mathbf{Q}} = \mathbf{N}_{\hat{\mathbf{Q}}\hat{\mathbf{U}}} \mathbf{M}_{\hat{\mathbf{U}}\hat{\mathbf{U}}}^{-1} \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}^T = \mathbf{N}_{\hat{\mathbf{Q}}\hat{\mathbf{U}}} \mathbf{B}_{\hat{\mathbf{U}}\mathbf{Q}}$$

$$\mathbf{B}_{\hat{\mathbf{Q}}\mathbf{U}} = \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{U}} - \mathbf{N}_{\hat{\mathbf{Q}}\hat{\mathbf{U}}} \mathbf{M}_{\hat{\mathbf{U}}\hat{\mathbf{U}}}^{-1} \mathbf{N}_{\mathbf{Q}\hat{\mathbf{U}}}^T \mathbf{N}_{\mathbf{Q}\mathbf{U}} = \mathbf{N}_{\hat{\mathbf{Q}}\mathbf{U}} + \mathbf{N}_{\hat{\mathbf{Q}}\hat{\mathbf{U}}} \mathbf{B}_{\hat{\mathbf{U}}\mathbf{U}}$$

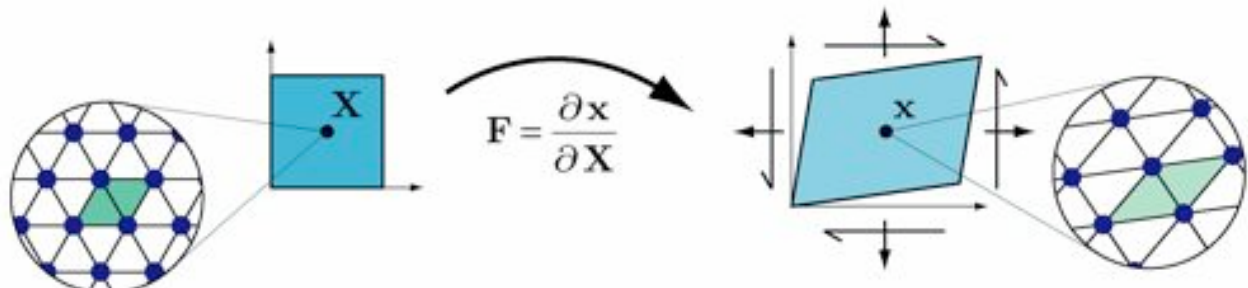
Coupled equilibrium equations and Cauchy-Born correction

The equations of static equilibrium are:

$$\mathbf{R}_Q = \frac{\partial \Pi}{\partial \mathbf{Q}} = \frac{\partial \Pi_Q}{\partial \mathbf{Q}} + \mathbf{B}_{\hat{\mathbf{Q}}\mathbf{Q}}^T \frac{\partial \Pi_Q}{\partial \hat{\mathbf{Q}}} + \mathbf{B}_{\hat{\mathbf{U}}\mathbf{Q}}^T \frac{\partial \Pi_U}{\partial \hat{\mathbf{U}}} - \mathbf{F}_Q = 0$$

$$\mathbf{R}_U = \frac{\partial \Pi}{\partial \mathbf{U}} = \frac{\partial \Pi_U}{\partial \mathbf{U}} + \mathbf{B}_{\hat{\mathbf{U}}\mathbf{U}}^T \frac{\partial \Pi_U}{\partial \hat{\mathbf{U}}} + \mathbf{B}_{\hat{\mathbf{Q}}\mathbf{U}}^T \frac{\partial \Pi_Q}{\partial \hat{\mathbf{Q}}} - \mathbf{F}_U = 0$$

Continuum strain energy is computed using the Cauchy-Born rule [Born (1940)]:



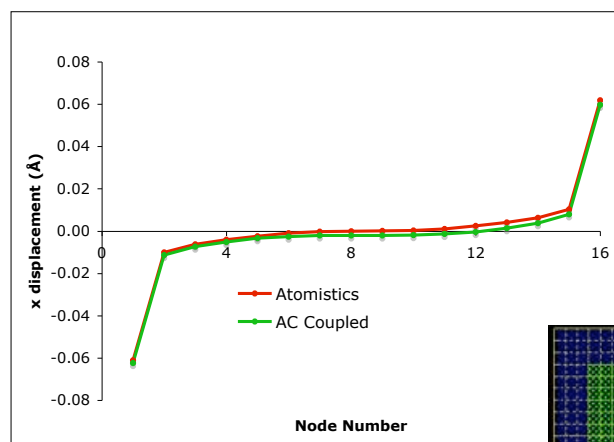
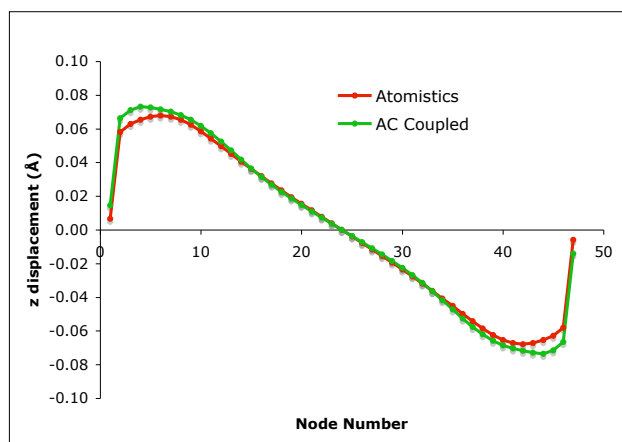
$$\begin{aligned} \Phi(\mathbf{F}) &= \frac{1}{V_0} \sum_i \varphi(r_{(i)}) \\ &= \frac{1}{V_0} \sum_i \varphi(\mathbf{R}_{(i)}, \mathbf{F}) \end{aligned}$$

For overlap elements, the energy from real atom - ghost atom bonds is present.

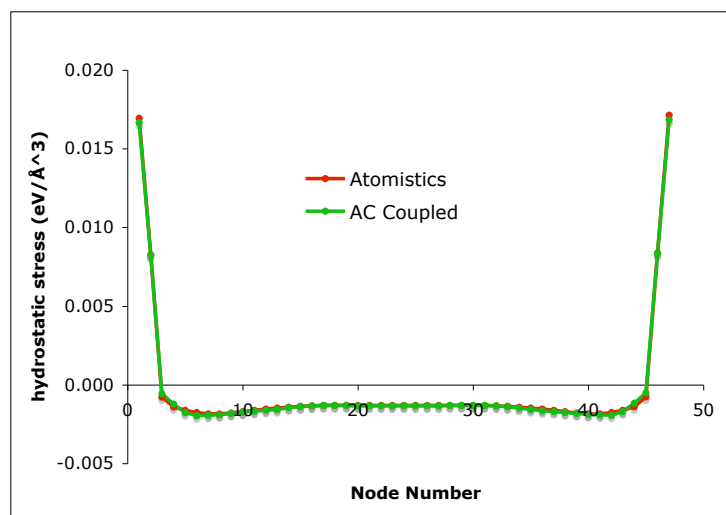
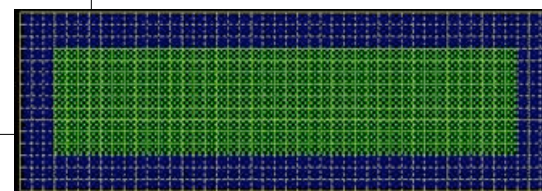
A density term must be introduced so that the Cauchy-Born rule used for these elements only accounts for the bonds that are not explicitly represented:

$$\Phi(\mathbf{F}) = \frac{1}{V_0} \sum_i \rho_{(i)} \varphi(r_{(i)}) = \frac{1}{V_0} \sum_i \rho_{(i)} \varphi(\mathbf{R}_{(i)}, \mathbf{F}) \quad 0 \leq \rho_{(i)}(\mathbf{X}) \leq 1$$

Surface relaxation of a [100] nanowire

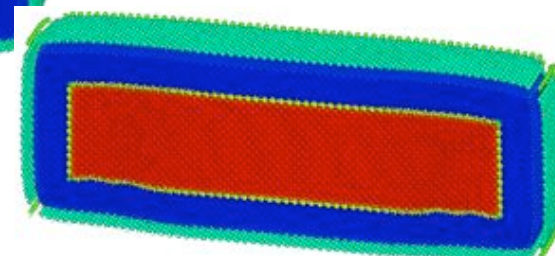


Ghost Atoms
Real Atoms



atomistic simulation

displacements
magnified by 100x



Quantifying stress in an atomistic simulation

Virial Theorem (Clausius, Maxwell 1870)

Cauchy stress

(time and ensemble average)

$$\boldsymbol{\sigma} = -\frac{1}{V} \left\langle \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{f}^{\alpha\beta} + \sum_{\alpha=1}^N m_{\alpha} \mathbf{v}^{\alpha} \otimes \mathbf{v}^{\alpha} \right\rangle$$

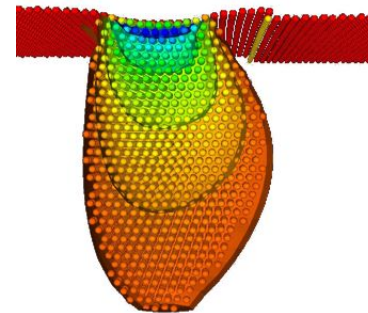
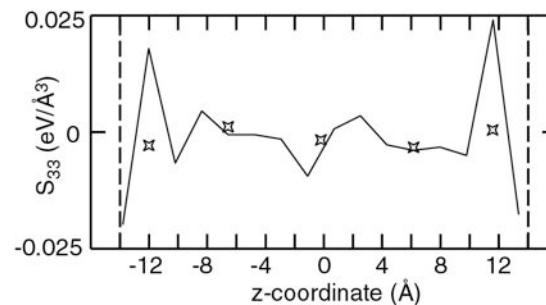
Virial stress

(local, instantaneous measure of stress)

$$\boldsymbol{\pi}^{\alpha} = -\frac{1}{V_{\alpha}} \left\{ \frac{1}{2} \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{f}^{\alpha\beta} + m_{\alpha} \mathbf{v}^{\alpha} \otimes \mathbf{v}^{\alpha} \right\} \quad \boldsymbol{\sigma} = \frac{1}{N} \left\langle \sum_{\alpha=1}^N \boldsymbol{\pi}^{\alpha} \right\rangle$$

Virial stress is NOT equivalent to (true) Cauchy stress:

1. “Static” continuum versus dynamic atoms.
2. Unphysical values are produced for non-symmetric arrangements of atoms, e.g. free surface.

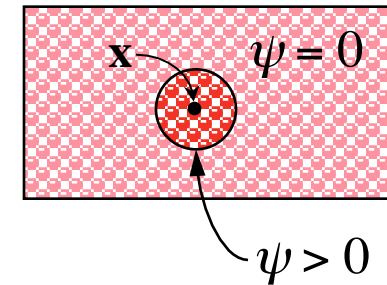


Atomistic-Continuum formulation of R.J. Hardy

Hardy (*Journal of Chemical Physics*, 1982) -

$$\rho(\mathbf{x}, t) = \sum_{\alpha=1}^N m^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \quad \mathbf{p}(\mathbf{x}, t) = \sum_{\alpha=1}^N m^{\alpha} \mathbf{v}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x})$$

$$E^0(\mathbf{x}, t) = \sum_{\alpha=1}^N \left\{ \frac{1}{2} m^{\alpha} \mathbf{v}^{\alpha} \cdot \mathbf{v}^{\alpha} + \phi^{\alpha} \right\} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \quad [\psi] \sim \frac{1}{V_c}$$



Applying these expressions to the spatial forms of the balance laws, *e.g.*

$$\frac{\partial \mathbf{p}}{\partial t} = \frac{\partial}{\partial \mathbf{x}} \cdot (\boldsymbol{\sigma} - \rho \mathbf{v} \otimes \mathbf{v}) \quad \text{linear momentum}$$

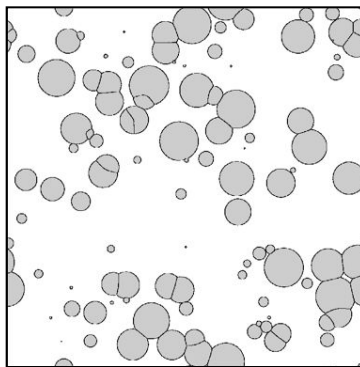
and separating continuum-scale momentum flux from atomic motion,

$$\hat{\mathbf{v}}^{\alpha}(\mathbf{x}, t) = \mathbf{v}^{\alpha}(t) - \mathbf{v}(\mathbf{x}, t) \quad \longleftarrow \quad \mathbf{v} \equiv \mathbf{p} / \rho$$

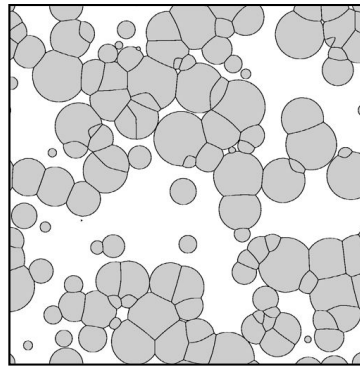
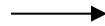
yields an expression for the Cauchy stress tensor:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = - \left\{ \frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{x}^{\alpha\beta} \otimes \mathbf{f}^{\alpha\beta} B^{\alpha\beta}(\mathbf{x}) + \sum_{\alpha=1}^N m^{\alpha} \hat{\mathbf{v}}^{\alpha} \otimes \hat{\mathbf{v}}^{\alpha} \psi(\mathbf{x}^{\alpha} - \mathbf{x}) \right\}$$

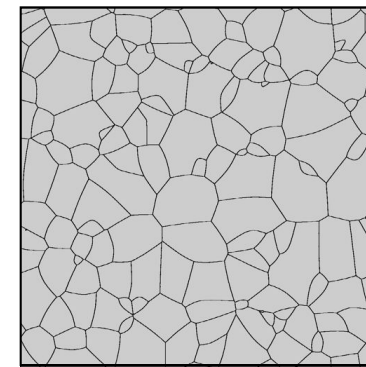
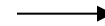
Example: Effect of stress during thin film growth



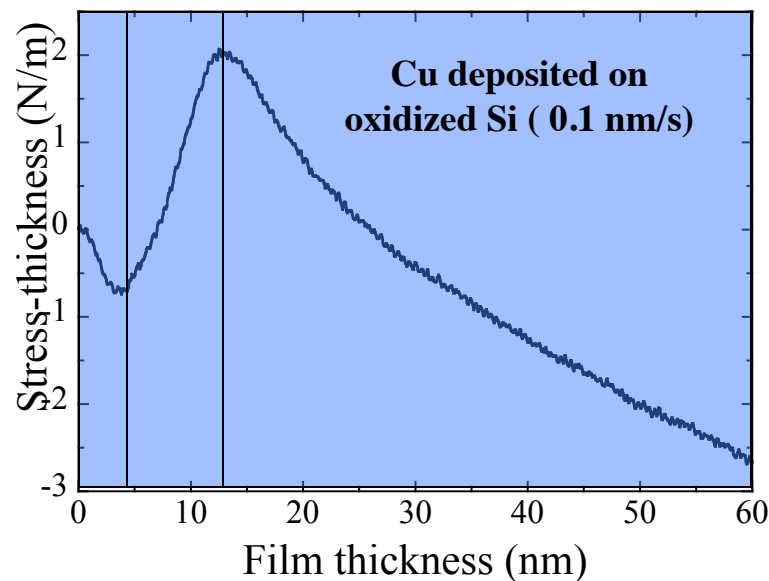
island nucleation



growth to impingement



film continuity



Experiment produces information on the average stress in the film only.

Questions that need to be answered:

How large is stress near coalescence region?

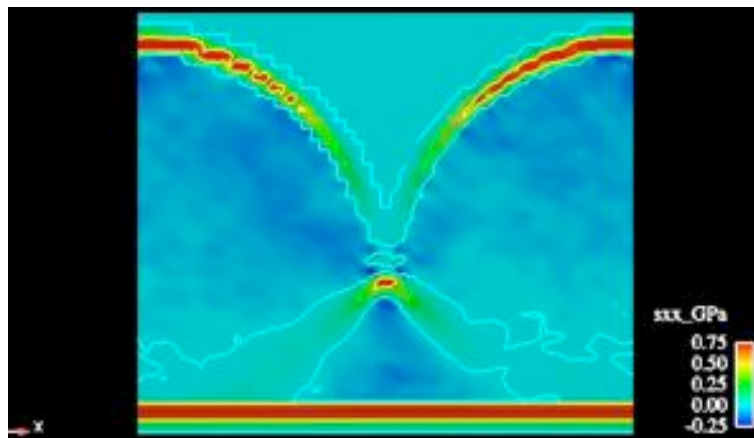
Does material yield occur, *i.e.* defects created?

How is stress distributed throughout the island structures?

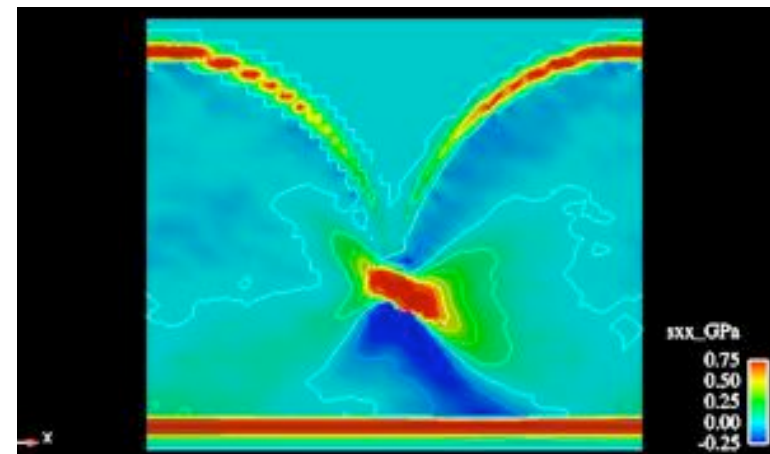
Example: Stress during island coalescence

Time-averaged Hardy stress analysis provides a stress map of isolated and coalesced islands:

Isolated



Post-coalescence



Significant observations:

- Analyses correlate material defects (dislocations, voids) with stress fields.
- Types of defects created depend on island size and deposition conditions.
- For smaller islands, tensile stress extends through system even after void formation.



Concluding Remarks

- What's next?
 - Atom-Continuum coupling for finite temperature and dynamics
 - Finite temperature: Wagner *et al.*, *CMAME*, 2008.
 - Develop material frame expressions for evaluation in atomistics

$$\mathbf{P} = -\frac{1}{2} \sum_{\alpha=1}^N \sum_{\beta \neq \alpha}^N \mathbf{f}^{\alpha\beta} \otimes \mathbf{X}^{\alpha\beta} B^{\alpha\beta}(\mathbf{X})$$

- Use of continuum fields for estimating \mathbf{J} , driving force for fracture
- Simulations performed using LAMMPS: <http://lammps.sandia.gov>
- Thank you to: Doug Bammann, Robert Hardy, Jeff Hoyt, Reese Jones, Patrick Klein, Jeremy Templeton and Ed Webb.
- For more information: jzimmer@sandia.gov